

# Stephan Ehrlich

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5551454/publications.pdf>

Version: 2024-02-01

13  
papers

54,380  
citations

686830

13  
h-index

1058022

14  
g-index

14  
all docs

14  
docs citations

14  
times ranked

45506  
citing authors

#	ARTICLE	IF	CITATIONS
1	Towards full Quantum-Mechanics-based Protein-Ligand Binding Affinities. ChemPhysChem, 2017, 18, 898-905.	1.0	46
2	A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. Physical Chemistry Chemical Physics, 2017, 19, 32184-32215.	1.3	1,230
3	Automated Transition State Search and Its Application to Diverse Types of Organic Reactions. Journal of Chemical Theory and Computation, 2017, 13, 5780-5797.	2.3	125
4	The frustrated Lewis pair pathway to methylene phosphonium systems. Chemical Science, 2014, 5, 797-803.	3.7	47
5	Accurate Thermochemistry for Large Molecules with Modern Density Functionals. Topics in Current Chemistry, 2014, , 1-23.	4.0	17
6	Dispersion-Corrected Density Functional Theory for Aromatic Interactions in Complex Systems. Accounts of Chemical Research, 2013, 46, 916-926.	7.6	330
7	Dispersion-Driven Conformational Isomerism in $\pi$ -Bonded Dimers of Larger Acenes. Angewandte Chemie - International Edition, 2013, 52, 10892-10895.	7.2	47
8	Splitting of dihydrogen by five-membered zirconacycloallene: a novel pathway to conjugated diene zirconocene complexes. Chemical Communications, 2012, 48, 11085.	2.2	16
9	A DFT-D study of structural and energetic properties of TiO <sub>2</sub> modifications. Journal of Physics Condensed Matter, 2012, 24, 424206.	0.7	51
10	On the Importance of the Dispersion Energy for the Thermodynamic Stability of Molecules. ChemPhysChem, 2011, 12, 1258-1261.	1.0	188
11	System-Dependent Dispersion Coefficients for the DFT-D <sub>3</sub> Treatment of Adsorption Processes on Ionic Surfaces. ChemPhysChem, 2011, 12, 3414-3420.	1.0	318
12	Effect of the damping function in dispersion corrected density functional theory. Journal of Computational Chemistry, 2011, 32, 1456-1465.	1.5	15,980
13	A consistent and accurate <i>ab initio</i> parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. Journal of Chemical Physics, 2010, 132, 154104.	1.2	35,972